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Supporting Information

Simultaneous Production of Psilocybin and a Cocktail of β-Carboline Monoamine Oxidase Inhibitors in “Magic” Mushrooms

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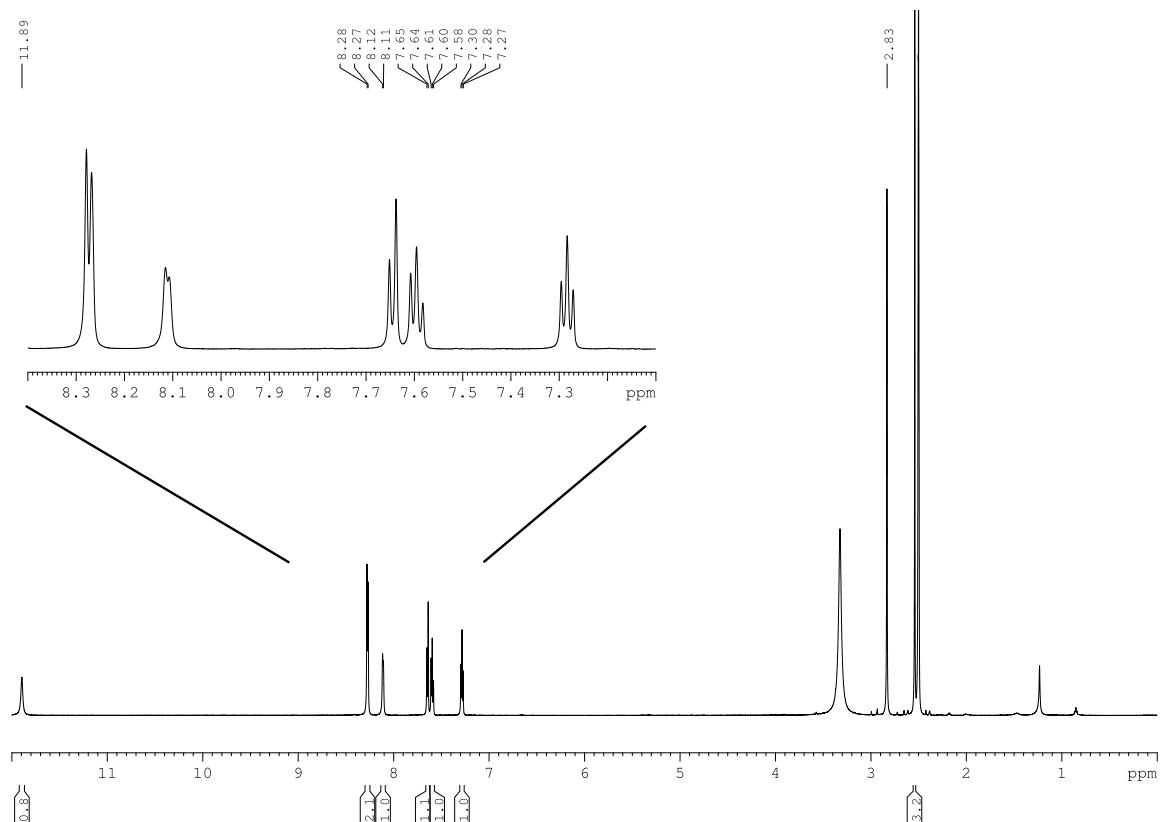


Figure S1. ^1H NMR spectrum of **4** in $\text{DMSO}-d_6$

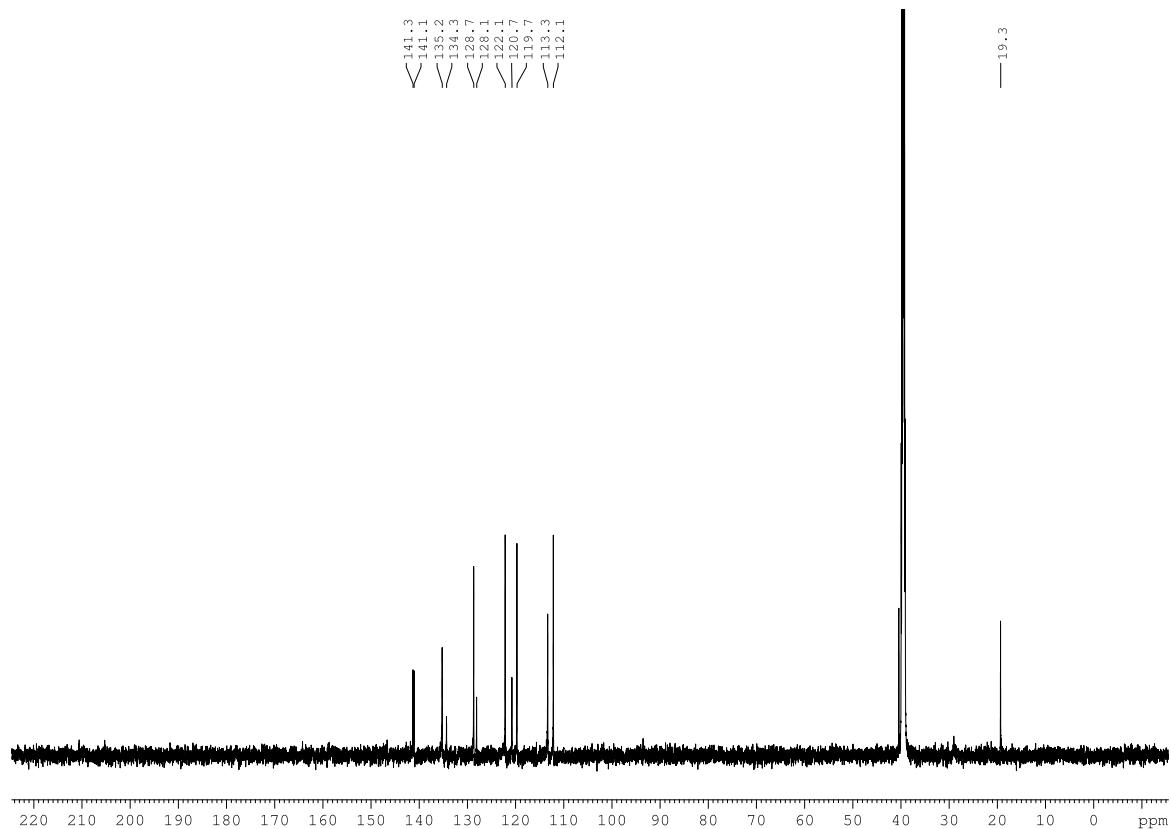


Figure S2. ^1H -decoupled ^{13}C NMR spectrum of **4** in $\text{DMSO}-d_6$

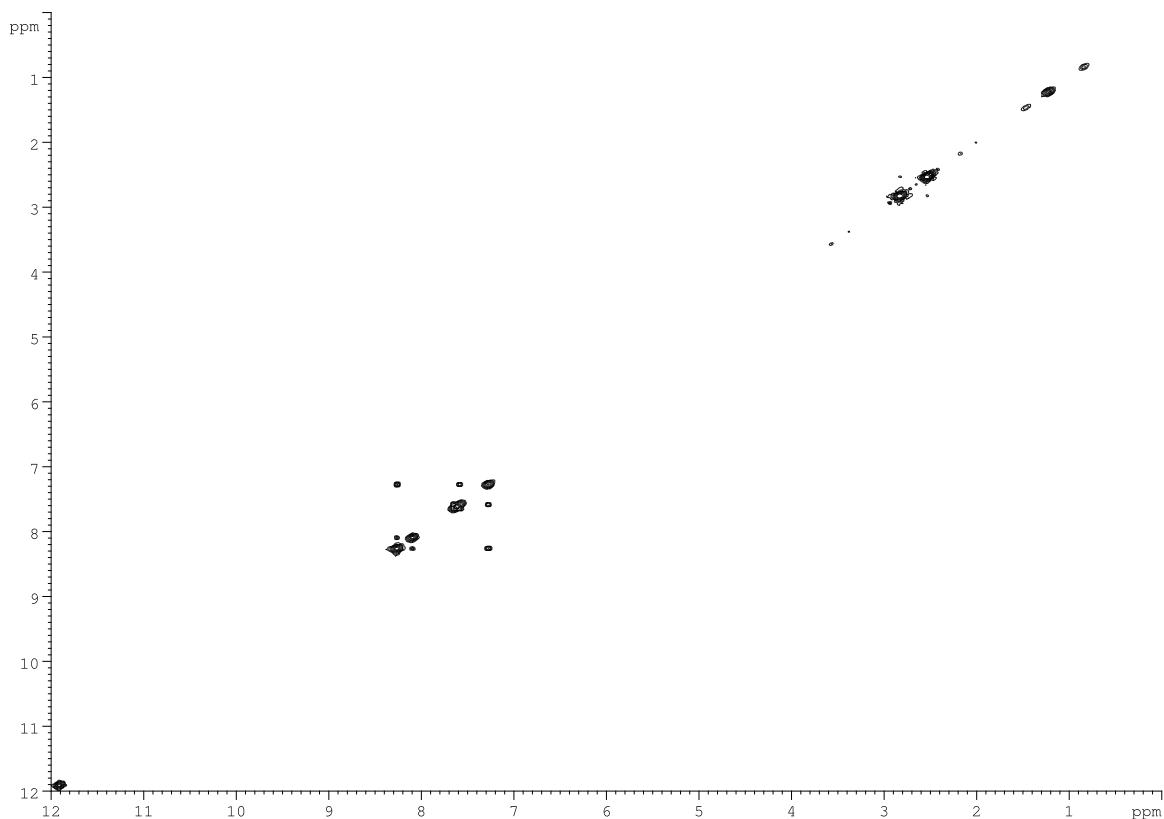


Figure S3. $^1\text{H},^1\text{H}$ COSY spectrum of **4** in $\text{DMSO}-d_6$

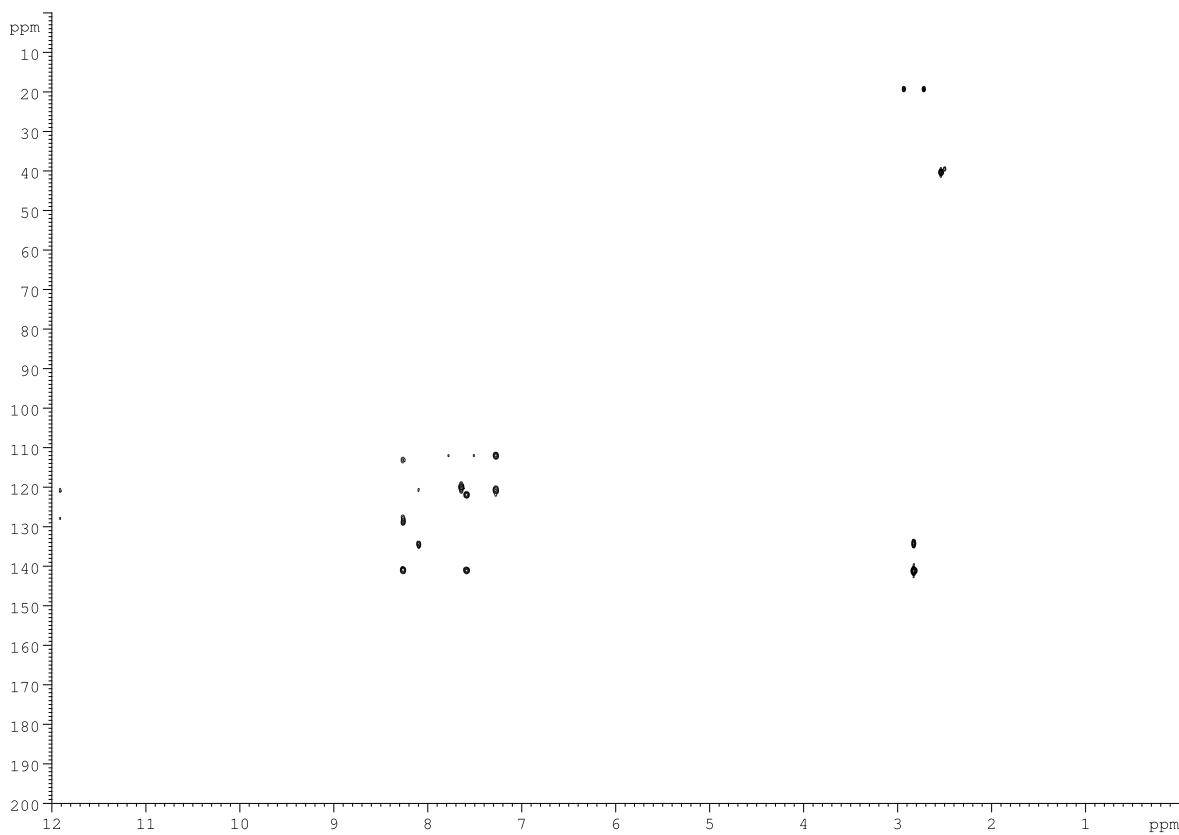


Figure S4. $^1\text{H},^{13}\text{C}$ HMBC spectrum of **4** in $\text{DMSO}-d_6$

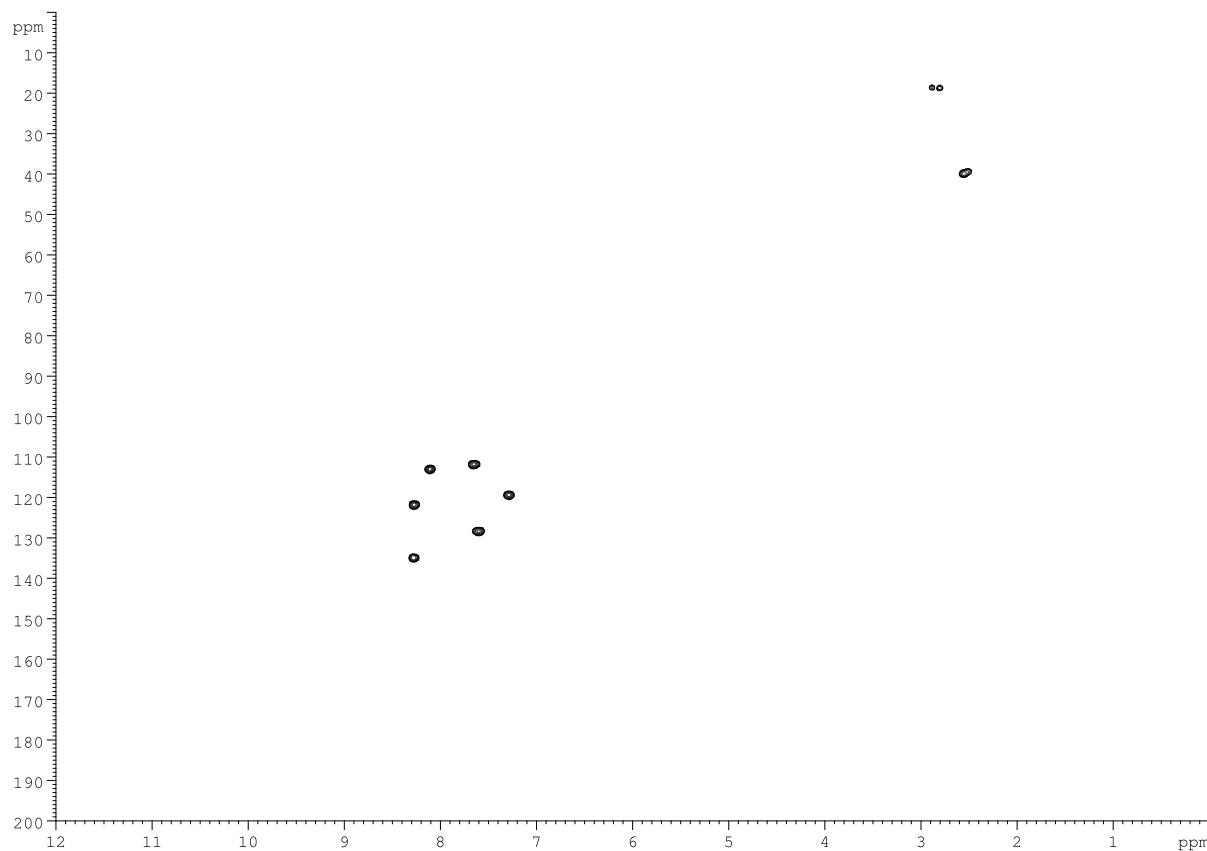


Figure S5. $^1\text{H}, ^{13}\text{C}$ HSQC spectrum of **4** in $\text{DMSO}-d_6$

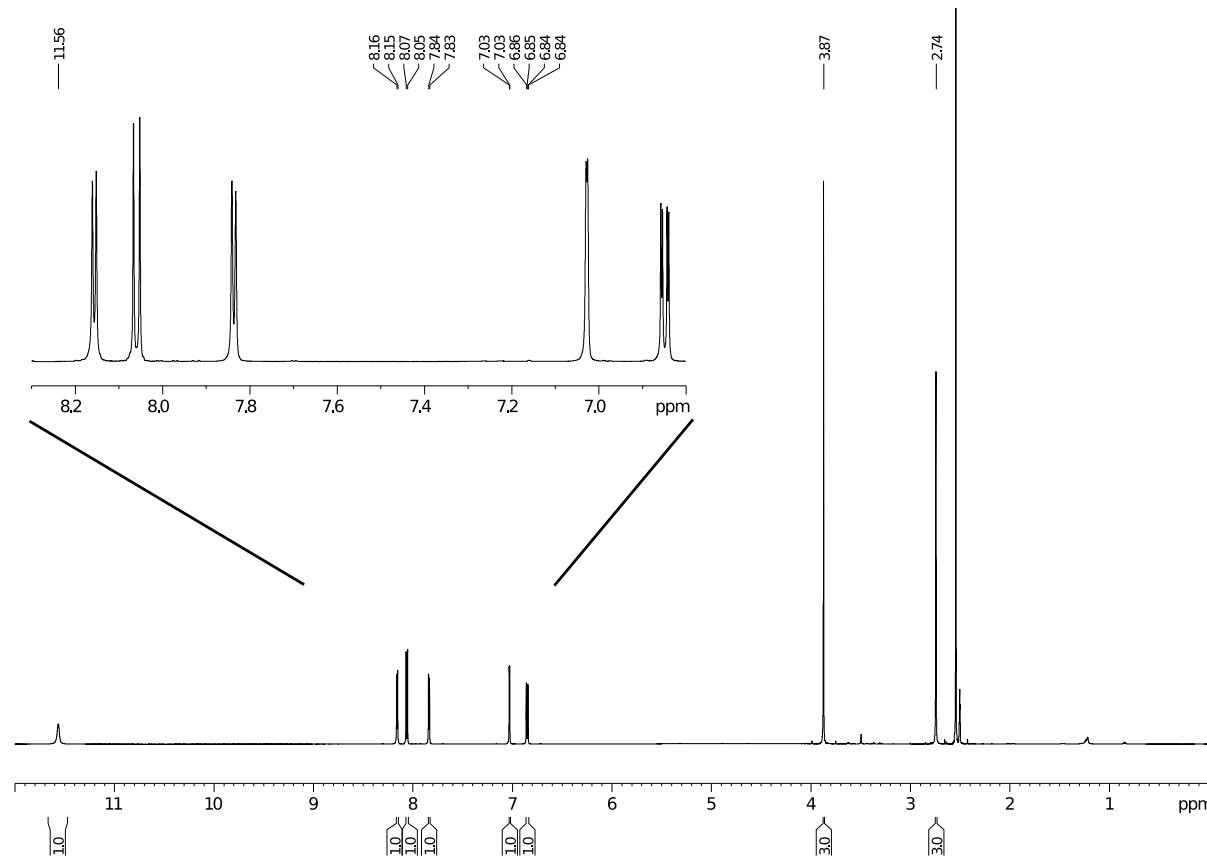


Figure S6. ^1H NMR spectrum of **5** in $\text{DMSO}-d_6$

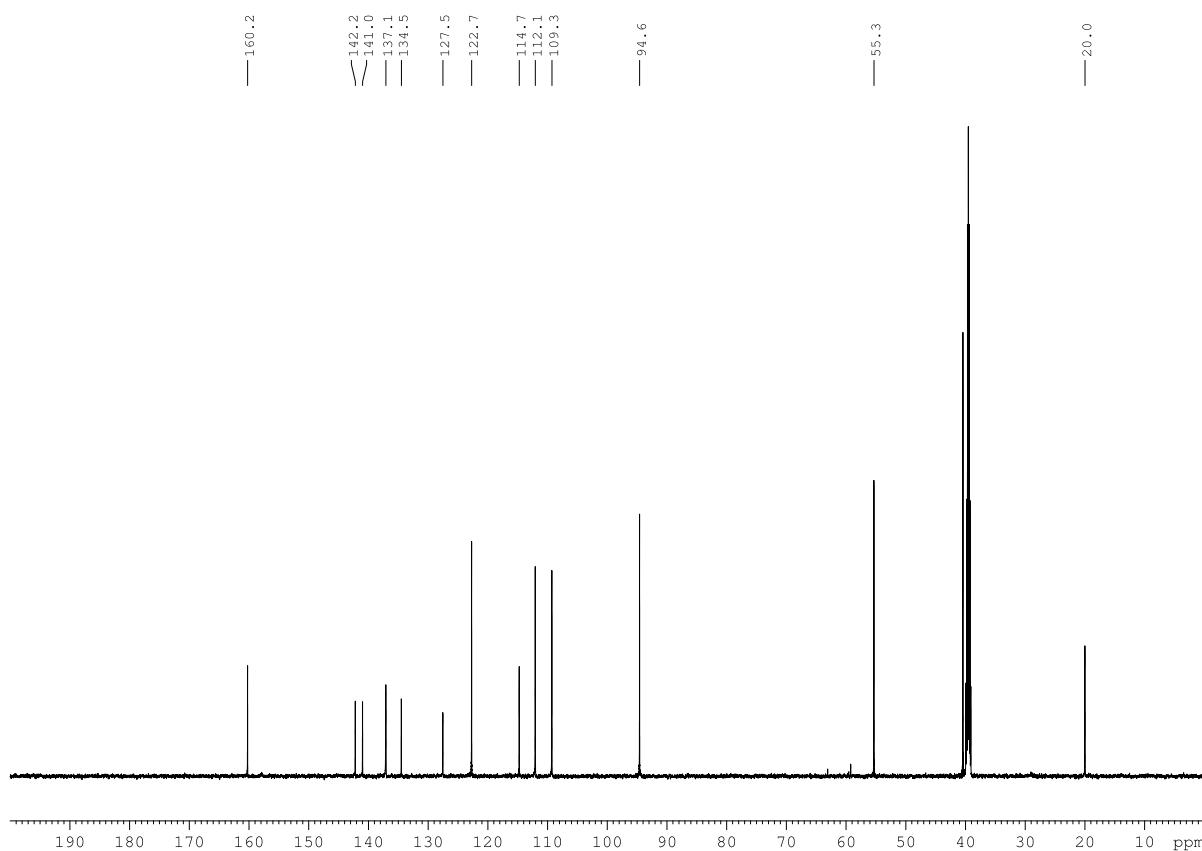


Figure S7. ^1H -decoupled ^{13}C NMR spectrum of **5** in $\text{DMSO}-d_6$

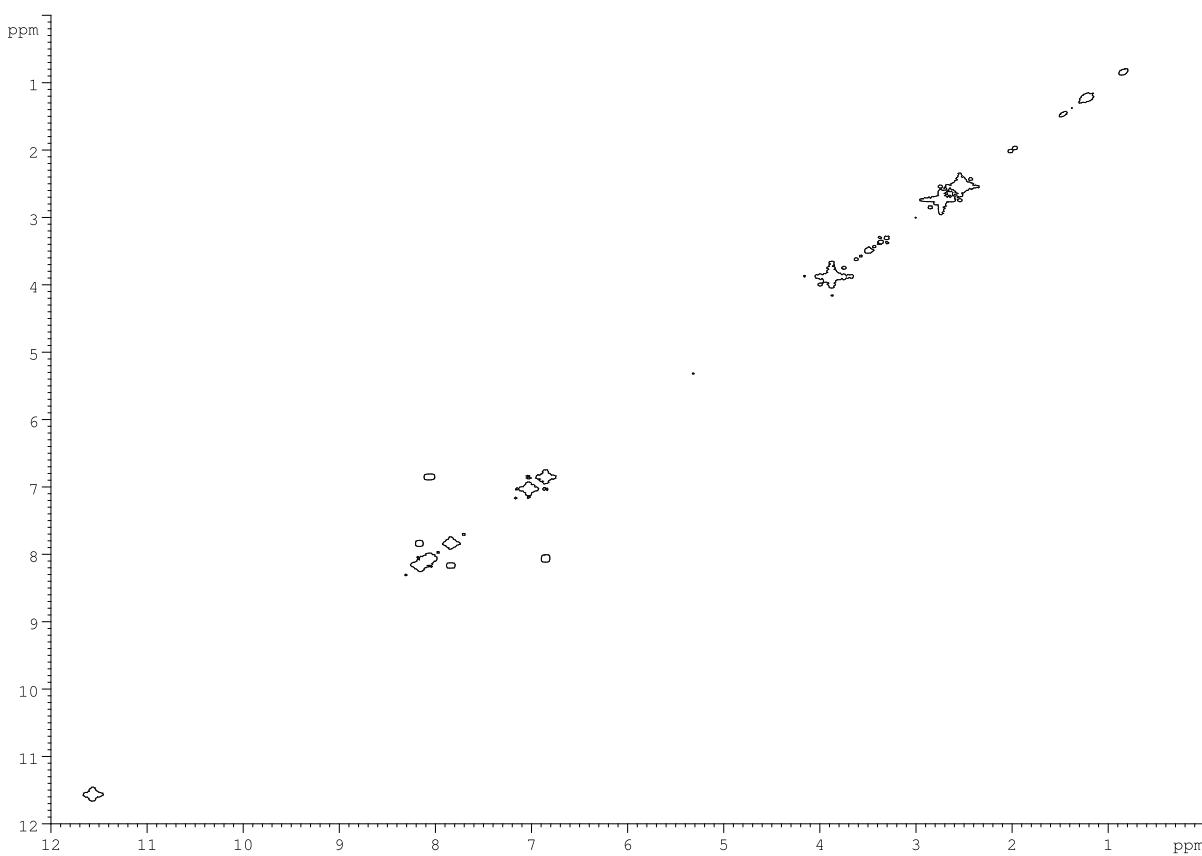


Figure S8. $^1\text{H},^1\text{H}$ COSY spectrum of **5** in $\text{DMSO}-d_6$

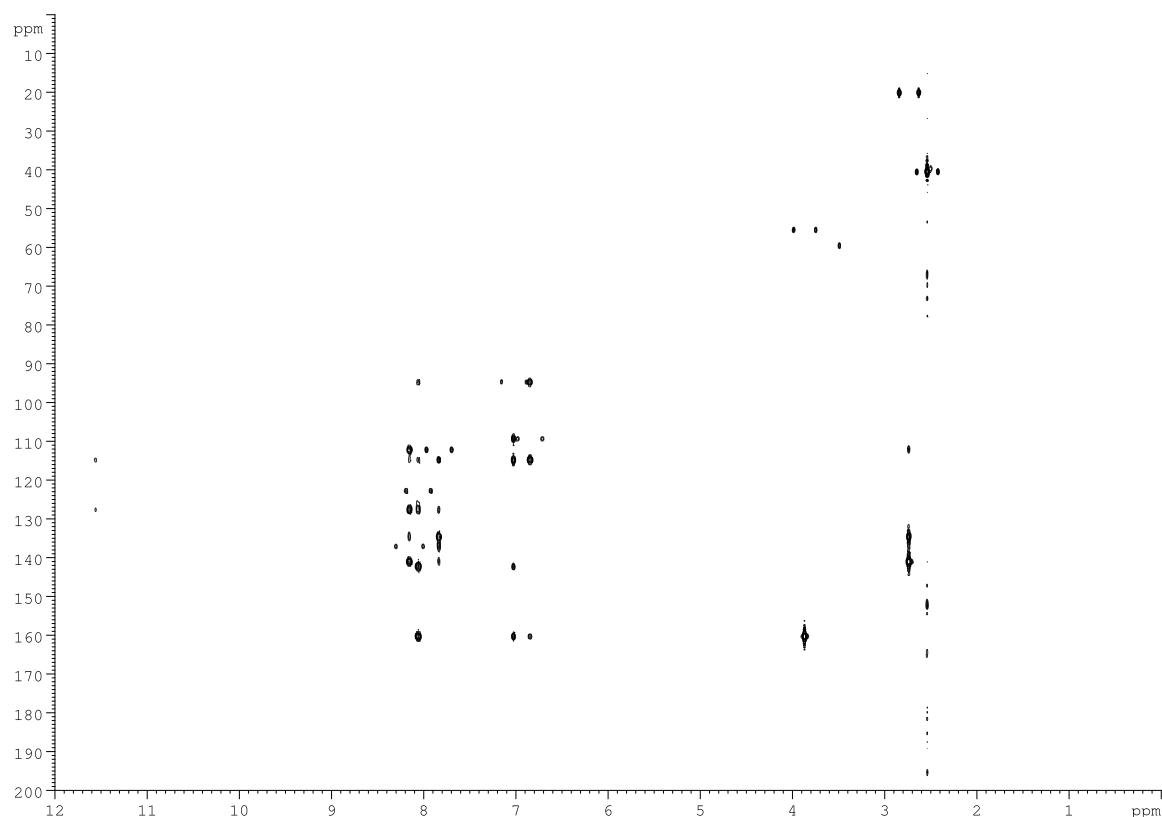


Figure S9. $^1\text{H},^{13}\text{C}$ HMBC spectrum of **5** in $\text{DMSO}-d_6$

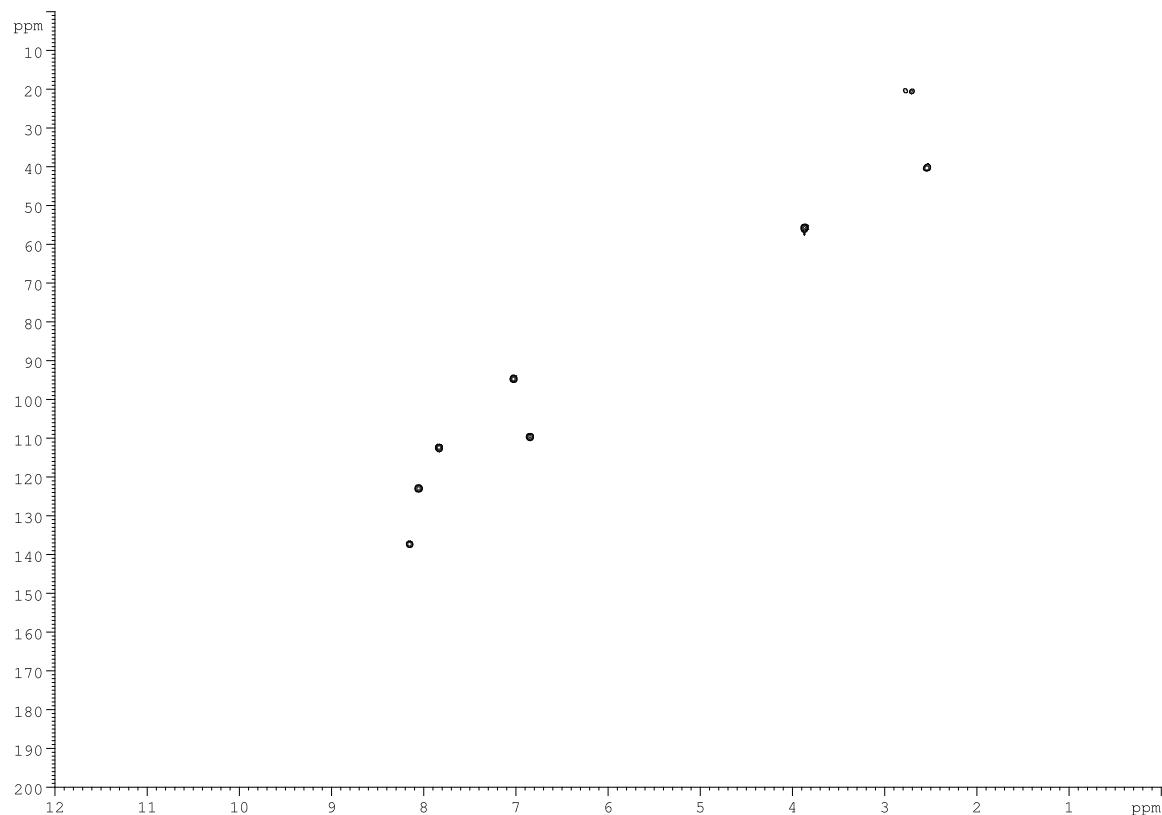
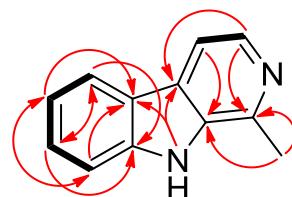
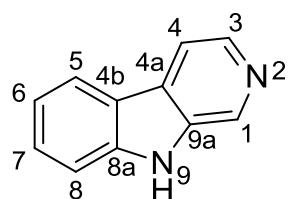


Figure S10. $^1\text{H},^{13}\text{C}$ HSQC spectrum of **5** in $\text{DMSO}-d_6$

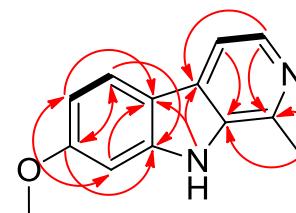
Table S1. NMR spectroscopic data of *Psilocybe* β-carbolines in DMSO-*d*₆. Numbering of positions, COSY (bold lines) and selected HMBC (red arrows) key correlations are shown below the table.

pos.	harmane (4)				harmine (5)			
	δ_c [ppm]	δ_h [ppm], M (J [Hz])	COSY ($^1H \rightarrow ^1H$)	HMBC ($^1H \rightarrow ^{13}C$)	δ_c [ppm]	δ_h [ppm], M (J [Hz])	COSY ($^1H \rightarrow ^1H$)	HMBC ($^1H \rightarrow ^{13}C$)
1	141.3	-			141.0	-		
2	-	-			-	-		
3	135.2	8.27, d (5.4)*	4	1, 4a	137.1	8.16, d (5.3)	4	1, 4, 4a
4	113.3	8.11, d (5.4)	3	4b, 9a	112.1	7.84, d (5.3)	3	3, 4b, 9a
4a	128.7	-			127.5	-		
4b	120.7	-			114.7	-		
5	122.1	8.28, d (8.0)*	6	7, 8a	122.7	8.06, d (8.6)	6	7, 4a, 8a
6	119.7	7.28, dd (8.0, 7.0)*	5, 7	4b, 8	109.3	6.85, dd (2.3, 8.6)	5	4b, 8
7	128.1	7.60, dd (8.2, 7.0)*	8, 6	5, 8a	160.2	-		
8	112.1	7.64, d (8.2)	7	4b, 6	94.6	7.03, d (2.0)		4b, 6, 7, 8a
8a	141.1	-			142.2	-		
9	-	11.89, s		4a, 4b	-	11.56, s		4a, 4b
9a	134.3	-			134.5	-		
CH ₃	19.3	2.83, s		1, 9a	55.3	3.87, s		7
OCH ₃	-	-	-	-	20.0	2.74, s		1, 9a

* coupling constants taken from sel-TOCSY (7.28 and 8.11 ppm).



harmane (4)



harmine (5)

Table S2. β -caroline concentrations in *Psilocybe cubensis* and *P. mexicana* ($\mu\text{g/g}$ dry mass).
harmane (4)

	<i>P. cubensis</i>	<i>P. mexicana</i>
carpophores	0.08	n.d.
mycelium	1.32	21.48
sclerotia	-	2.01

harmine (5)

	<i>P. cubensis</i>	<i>P. mexicana</i>
carpophores	0.10	0.04
mycelium	0.08	0.61
sclerotia	-	1.62

Table S3. *Psilocybe* strains used in this study.

Species	Isolate	Nuclear state	Material analyzed
<i>P. cubensis</i> ^[1]	FSU12407	dikaryon	cultivated carpophores, mycelium
<i>P. cubensis</i> ^[1]	FSU12410	dikaryon	cultivated carpophores
<i>P. cyanescens</i>	FSU12414	dikaryon	collected carpophores
<i>P. semilanceata</i>	FSU13616	dikaryon	collected carpophores
<i>P. mexicana</i>	FSU13617	dikaryon	cultivated carpophores, sclerotia, mycelium

[1] C. Lenz, J. Wick, D. Hoffmeister, *J. Nat. Prod.* **2017**, *80*, 2835-2838.